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GRAPH DECONVOLUTION METHODS FOR DIRECTED LIGAND GENERATION

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Modern therapy becomes more and more target. This is caused by both number of novel targets and personal medicine approach. To achieve high effectivity of treatment novel combinations of high-selective target drugs should be found. In these conditions drug design and discovery have to be cheaper and faster to refrain treatment cost in admissible boundaries.

In vitro screening cannot satisfy these requirements due measure any more. Unfortunately blind *in silico* screening of multimillion combinatorial libraries cannot guarantee high successful rate since it often optimize just ligand-protein binding, but not ADME(T) or synthesis possibility. So drug designers have to find a new approach, that may become a gamechanger in the field. One of most likely candidates to this role is feature-based directed structure generation.

To achieve good generation results with good generation-experiment correlation a good vector compression of molecule should be used. This lets to use modern machine learning techniques that require linear vector spaces to work with. Sad fact is that vectorizing and especially devectorizing of arbitrary graph is an unsolved problem. In this talk we want to highlight some approaches for this task and results, that can be achieved by using these approaches.

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